Micro-Scale Simulation of Adsorption-Diffusion Behaviors of Nanoparticles onto Oil/Water Interface

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Abstract

A novel, hybrid pore-scale simulation method using Lattice-Boltzmann (LB) coupled with Langevin-Dynamics (LD) is proposed to investigate the physics of nanoparticles onto oil/water interface. By the means of the new LB-LD coupling model, the adsorption and diffusion characterization of nanoparticles onto oil/water interface are investigated. Moreover, by introducing interference coefficient and non-equilibrium time, a modified Langmuir adsorption equation is first established by more accurately quantifying the adsorption characterization of nanoparticles and the consequent impacts onto oil/water interfacial tension, of which the classical Langmuir adsorption equation cannot take account. For a target representative example of SiO2 nanoparticles, it is observed that small-size nanofluids with high concentration could accelerate the adsorption of nanoparticles and therefore help decrease oil/water interface tension. In addition, both the lateral and longitudinal diffusion coefficients of nanoparticles into the water phase and onto oil/water interface are obtained, and of which the underlying mechanisms are explained in details.

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